Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2,2-Triphenyl-*N*-(2-pyridylmethyl)acetamide

Laura R. Whiteaker, Urmila Pal Chaudhuri, Douglas R. Powell and Robert P. Houser*

Department of Chemistry and Biochemistry, University of Oklahoma, 620 Parrington Oval, Room 208, Norman, OK 73019-3051 USA

Correspondence e-mail: houser@ou.edu

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.092
Data-to-parameter ratio = 14.7

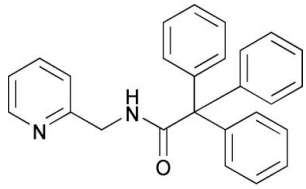
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 29 June 2006
Accepted 5 July 2006

The title compound, $C_{26}H_{22}N_2O$, possesses normal geometric parameters and forms centrosymmetric dimeric associations *via* N—H···N hydrogen bonds.

Comment

In the preceding paper (Whiteaker *et al.* 2006), we described the crystal structure of the related phenylmethyl-substituted pyridyl amide, $C_{14}H_{14}N_2O$, (I). Here we present the crystal structure of the triphenylmethyl-substituted title compound (II). Compound (II) (Fig. 1) possesses normal geometric parameters. The hydrogen-bonding scheme in (II) (Table 1) features an N—H···N interaction; inversion symmetry generates a dimeric association of molecules *via* two such bonds (Fig. 2).



(II)

The hydrogen-bonding scheme in (I) is different and involves N—H···O bonds leading to one-dimensional chains of molecules. This difference may arise for steric reasons; the

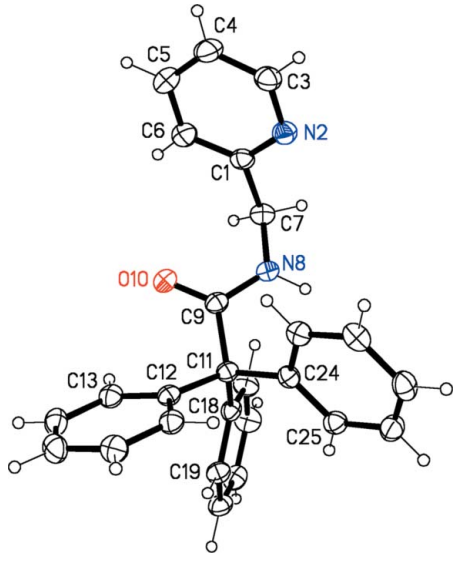


Figure 1
View of (II) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

bulky triphenylmethyl group in (II) prevents the amide groups from getting close enough to form the hydrogen-bonded chains that occur in (I).

Experimental

Compound (II) was synthesized according to the previously reported procedure (Pal Chaudhuri *et al.*, 2006). X-ray quality crystals of (II) were grown by vapor diffusion of diethyl ether into a dichloromethane solution of (II).

Crystal data

$C_{26}H_{22}N_2O$
M_r = 378.46
Monoclinic, $P2_1/n$
a = 8.6013 (11) Å
b = 17.895 (2) Å
c = 13.4072 (17) Å
β = 106.657 (2)°
V = 1977.0 (4) Å^3
Z = 4
D_x = 1.271 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 (2) K
Block, brown
0.58 × 0.45 × 0.35 mm

Data collection

Bruker APEX CCD diffractometer
ω scans
Absorption correction: multi-scan *SADABS* (Sheldrick, 2002)
T_{min} = 0.956, T_{max} = 0.973
20831 measured reflections
3897 independent reflections
3660 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.092
S = 1.01
3897 reflections
266 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 0.7P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0262 (18)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N8—H8···N2^{i}	0.903 (14)	2.081 (14)	2.9544 (14)	162.4 (12)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

The C-bound H atoms were placed in idealized locations (C—H = 0.95–0.99 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The N-bound H atom was located in a difference map and its position was refined freely with U_{iso}(H) = 1.2U_{eq}(N).

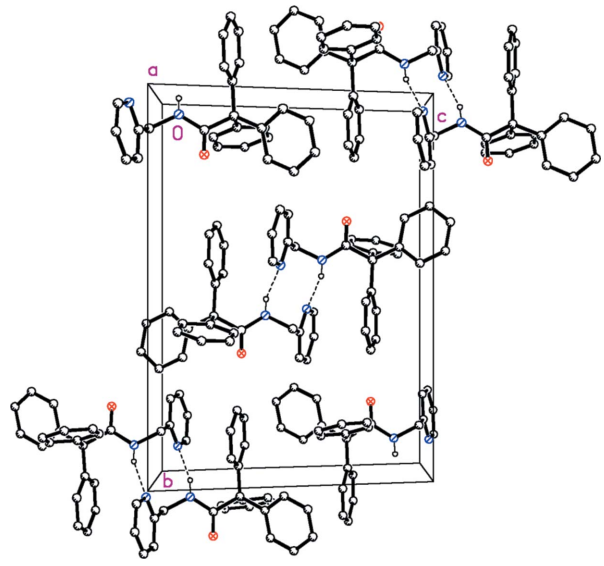


Figure 2
The molecular packing of (II), viewed along the *a* axis. H atoms have been omitted for clarity, except for those involved in hydrogen bonds (dashed lines).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

This work was supported by the NSF (CHE-0094079) and the Herman Frasch Foundation. The authors also thank the NSF (CHE-0130835) and the University of Oklahoma for funds to acquire the CCD diffractometer and computers.

References

Bruker (1998). *SMART* and *SAINT*, Bruker AXS Inc., Madison, Wisconsin, USA.
Pal Chaudhuri, U., Whiteaker, L. R., Yang, L. & Houser, R. P. (2006). *Dalton Trans.* 1pp. 902–1908.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2002). *SADABS*. Version 2.03. University of Göttingen, Germany.
Whiteaker, L., Pal Chaudhuri, U., Powell, D. & Houser, R. P. (2006). *Acta Cryst.* E**62**, o3337–o3338.